Author Index to Volume 174

Aarts, J.F.M., see P.A. Hatherly 174 (1993) 453
Aben, I., see W. Ubachs 174 (1993) 285
Adamovich, I., see S. Saupe 174 (1993) 219
Agreiter, J., see B.E. Wurfel 174 (1993) 255
Ågren, H., see V. Carravetta 174 (1993) 141
Aguilar, M., R. Bianco, S. Miertus, M. Persico and J. Tomasi, Chemical reactions in solution: modelling of the delay of solvent synchronism (dielectric friction) along the reaction path of an S_N2 reaction 174 (1993) 397
Amaee, B. and W. Byers Brown, Exponential-α:6 potential parameters from ab initio calculations for atom–molecule interactions 174 (1993) 351
Andersson, L.L., J. Davidsson and S. Nordholm, A molecular dynamics investigation of energy transfer efficiency in collisions of diatomic molecules 174 (1993) 111

Banichevich, A. and S.D. Peyerimhoff, Theoretical study of the ground and excited states of ozone in its symmetric nuclear arrangement 174 (1993) 93
Berden, G., W.L. Meerts and W. Kreiner, High-resolution laser-induced fluorescence and microwave–ultraviolet double resonance spectroscopy on 1-cyanonaphthalene 174 (1993) 247
Berden, G., see D. Consalvo 174 (1993) 267
Bergman, R.C., see S. Saupe 174 (1993) 219
Berthier, G., see F. Pauzat 174 (1993) 71
Beumee, J.G.B., see M.H. Lissak 174 (1993) 1
Bianco, R., see M. Aguilar 174 (1993) 397
Billard, I., see F. Didierjean 174 (1993) 331
Boldyrev, A.I., see V.G. Zakrzewski 174 (1993) 167
Bondybey, V.E., see B.E. Wurfel 174 (1993) 255
Broo, A., The dynamics of some metal–organic and organic molecules in water solution studied by molecular mechanical and molecular dynamical methods 174 (1993) 127
Byers Brown, W., see B. Amaee 174 (1993) 351

Carravetta, V., Y. Luo and H. Ågren, Accurate photoionization cross sections of diatomic molecules by multi-configuration linear response theory 174 (1993) 141
Chen, C.H., see M.P. McCann 174 (1993) 417
Codling, K., see J.C. Creasey 174 (1993) 441
Codling, K., see P.A. Hatherly 174 (1993) 453
Consalvo, D., M. Drabbels, G. Berden, W.L. Meerts, D.H. Parker and J. Reuss, High-resolution laser-induced fluorescence study of a cage molecule, 1,4-diazabicyclo-[2,2,2]octane, DABCO 174 (1993) 267
Creasey, J.C., H.M. Jones, D.M. Smith, R.P. Tuckett, P.A. Hatherly, K. Codling and I. Powis, Fragmentation of valence electronic states of CF_4^+ and SF_6^+ studied by threshold photoelectron–photoion coincidence spectroscopy 174 (1993) 441

Datskou, I., see M.P. McCann 174 (1993) 417
Davidsson, J., see L.L. Andersson 174 (1993) 111
Deal, M., A. Gharvai, G.L. McPherson, C.E. Martinez and M.F. Herman, Scaling analysis of exciton annihilations in highly anisotropic crystals 174 (1993) 81
Decleva, P., see G. Fronzoni 174 (1993) 57
De Lange, M.C.C., D.T. Leeson, K.A.B. van Kuijk, A.H. Huizer and C.A.G.O. Varma, On the source of the anomalous fluorescence of 4-(dialkylamino)benzonitrile in aromatic hydrocarbon solvents: the role of exciplexes 174 (1993) 425
Devore, T.C. and J.L. Gole, Fluorine hot atom oxidation of bismuth vapor. A comment on the evaluation of the BiF bond energy 174 (1993) 409
Didierjean, F., I. Billard, W.F. Magalhaes and G. Duplâtre, Energetic states of positronium in liquids from the study of magnetic field effects and of spin conversion reactions 174 (1993) 331
Dietz, F., see N. Tyutyulkov 174 (1993) 343
Drabbels, M., see D. Consalvo 174 (1993) 267
Duplâtre, G., see F. Didierjean 174 (1993) 331
Dutt, A.K., Equilibrium and nonequilibrium steady states in the reversible Oregonator model (Chem. Phys. 162 (1992) 265). Erratum 174 (1993) 155

Ellinger, Y., see F. Pauzat 174 (1993) 71
Engler, C., see R. Neumann 174 (1993) 377
Evans, S., see M.P. McCann 174 (1993) 417

Fritzsche, S., R. Haberlandt, J. Kärger, H. Pfeifer and K. Heinzinger, On the diffusion mechanism of methane in a cation-free zeolite of type ZK4 174 (1993) 229
Fronzoni, G., P. Decleva and A. Lisini, Ab initio CI calculation of K shell absorption spectra in transition metal compounds 174 (1993) 57

Gabriel, W., P. Rosmus, K. Yamashita, K. Morokuma and P. Palmieri, Theoretical rotational–vibrational spectrum of SiH_2 ($X\ ^1A_1$ and $a\ ^3B_1$) 174 (1993) 45
Gérin, M., see F. Pauzat 174 (1993) 71
Gharvai, A., see M. Deal 174 (1993) 81
Gole, J.L., see T.C. Devore 174 (1993) 409
Grassi, M.J., see S. Saupe 174 (1993) 219

Haberlandt, R., see S. Fritzsche 174 (1993) 229
Hatherly, P.A., see J.C. Creasey 174 (1993) 441
Hatherly, P.A., K. Codling, D.M. Smith, R.P. Tuckett, K.R. Yoxall and J.F.M. Aarts, Radiative decay of the $\tilde{C}\ ^2T_2$ state of CF_4^+ measured by threshold photoelectron–fluorescence coincidence spectroscopy 174 (1993) 453
Heinzinger, K., see S. Fritzsche 174 (1993) 229
Herman, M.F., see M. Deal 174 (1993) 81
Hogervorst, W., see W. Ubachs 174 (1993) 285
Huizer, A.H., see M.C.C. de Lange 174 (1993) 425

Jones, H.M., see J.C. Creasey 174 (1993) 441
Joyeux, M., Vibrational chaos: rational tori, separatrices and Lyapunov exponents 174 (1993) 157

Kärger, J., see S. Fritzsche 174 (1993) 229
Klemp, D., see B. Nickel 174 (1993) 297
Klemp, D., see B. Nickel 174 (1993) 319
Kopelman, R., see L. Li 174 (1993) 367
Kreiner, W., see G. Berden 174 (1993) 247

Lask, G.M., see B.E. Wurfel 174 (1993) 255
Leeson, D.T., see M.C.C. de Lange 174 (1993) 425
Li, L. and R. Kopelman, Influence of external steady source structure on particle distributions and kinetics of diffusion-limited reactions. II. A+B→0 simulations 174 (1993) 367
Lisini, A., see G. Fronzoni 174 (1993) 57
Lissak, M.H., J.D. Sensabaugh, C.D. Schwieters, J.G.B. Beumee and H. Rabitz, Optimal control of classical anharmonic molecules represented with piecewise harmonic potential surfaces: analytic solution and selective dissociation of triatomic systems 174 (1993) 1
Luo, Y., see V. Carravetta 174 (1993) 141

Macheret, S.O. and J.W. Rich, Nonequilibrium dissociation rates behind strong shock waves: classical model 174 (1993) 25
Magalhaes, W.F., see F. Didierjean 174 (1993) 331
Martinez, C.E., see M. Deal 174 (1993) 81
Matyushov, D.V., Reorganization energy of electron transfer in polar liquids. Dependence on reactant size, temperature and pressure 174 (1993) 199
McCann, M.P., C.H. Chen, I. Datskou and S. Evans, Two-photon spectroscopy of molecular oxygen 174 (1993) 417
McPherson, G.L., see M. Deal 174 (1993) 81
Meerts, W.L., see G. Berden 174 (1993) 247
Meerts, W.L., see D. Consalvo 174 (1993) 267
Miertus, S., see M. Aguilar 174 (1993) 397
Milan, J.B., see W. Ubachs 174 (1993) 285
Millie, P., see C. Winter 174 (1993) 177
Millie, P., see C. Winter 174 (1993) 191
Morokuma, K., see W. Gabriel 174 (1993) 45

Neumann, R. and C. Engler, Quantum-statistical transition probabilities in diabatic 2D-potential surfaces. Influence of coupling in the potential terms 174 (1993) 377
Nickel, B. and D. Klemp, The lowest triplet state of azulene-h_8 and azulene-d_8 in liquid solution. I. Survey, kinetic considerations, experimental technique, and temperature dependence of triplet decay 174 (1993) 297
Nickel, B. and D. Klemp, The lowest triplet state of azulene-h_8 and azulene-d_8 in liquid solution. II. Phosphorescence and E-type delayed fluorescence 174 (1993) 319
Niedzielski, J., see J. Turulski 174 (1993) 387
Nordholm, S., see L.L. Andersson 174 (1993) 111

Osintsev, A.M., P.A. Purtov and K.M. Salikhov, Calculation of SNP effects in weak magnetic fields 174 (1993) 237

Palmieri, P., see W. Gabriel 174 (1993) 45

Parker, D.H., see D. Consalvo 174 (1993) 267
Pauzat, F., Y. Ellinger, G. Berthier, M. Gérin and Y. Viala, Theoretical study of a basic process in interstellar nitrogen chemistry: reaction of N with OH 174 (1993) 71
Persico, M., see M. Aguilar 174 (1993) 397
Peyerimhoff, S.D., see A. Banichevich 174 (1993) 93
Pfeifer, H., see S. Fritzsche 174 (1993) 229
Powis, I., see J.C. Creasey 174 (1993) 441
Purtov, P.A., see A.M. Osintsev 174 (1993) 237

Rabitz, H., see M.H. Lissak 174 (1993) 1
Reuss, J., see D. Consalvo 174 (1993) 267
Rich, J.W., see S.O. Macheret 174 (1993) 25
Rich, J.W., see S. Saupe 174 (1993) 219
Røeggen, I., see P. Wind 174 (1993) 345
Rosmus, P., see W. Gabriel 174 (1993) 45

Sakimoto, K., see J. Turulski 174 (1993) 387
Salikhov, K.M., see A.M. Osintsev 174 (1993) 237
Saupe, S., I. Adamovich, M.J. Grassi, J.W. Rich and R.C. Bergman, Vibrational and electronic excitation of nitric oxide in optical pumping experiments 174 (1993) 219
Schallmoser, G., see B.E. Wurfel 174 (1993) 255
Schlachta, R., see B.E. Wurfel 174 (1993) 255
Schleyer, P. von R., see V.G. Zakrzewski 174 (1993) 167
Schwieters, C.D., see M.H. Lissak 174 (1993) 1
Sensabaugh, J.D., see M.H. Lissak 174 (1993) 1
Smirnov, Y.M., Dissociative excitation of lithium atoms in collisions of electrons with LiCl molecules 174 (1993) 277
Smith, D.M., see J.C. Creasey 174 (1993) 441
Smith, D.M., see P.A. Hatherly 174 (1993) 453
Somsen, G.J., see W. Ubachs 174 (1993) 285
Stuiver, A.G., see W. Ubachs 174 (1993) 285

Thoma, A., see B.E. Wurfel 174 (1993) 255
Tomasi, J., see M. Aguilar 174 (1993) 397
Tuckett, R.P., see J.C. Creasey 174 (1993) 441
Tuckett, R.P., see P.A. Hatherly 174 (1993) 453
Turulski, J., J. Niedzielski and K. Sakimoto, The rate of ion-linear dipole capture at extremely low temperatures estimated with the use of the statistical adiabatic channel model 174 (1993) 387
Tyutyulkov, N. and F. Dietz, Energy gap equation of 1D polycondensed π-systems in the Hubbard approximation (Chem. Phys. 171 (1993) 293). Erratum 174 (1993) 343

Ubachs, W., I. Aben, J.B. Milan, G.J. Somsen, A.G. Stuiver and W. Hogervorst, Radiative and collisional relaxation of a single rovibrational quantum state of I_2: $E(0_g^+)$, $v=8$, $J=56$ 174 (1993) 285

Van Kuijk, K.A.B., see M.C.C. de Lange 174 (1993) 425
Varma, C.A.G.O., see M.C.C. de Lange 174 (1993) 425

Viala, Y., see F. Pauzat 174 (1993) 71
Von Niessen, W., see V.G. Zakrzewski 174 (1993) 167

Wind, P. and I. Røeggen, A theoretical study of the $(H_2)_2$ dimer. III. The isotropic potential 174 (1993) 345
Winter, C. and P. Millie, Theoretical study of small hydrogenated silicon compounds. I. Theoretical study of the SiH_2 dissociation channels up to 8 eV excitation energy 174 (1993) 177
Winter, C. and P. Millie, Theoretical study of small hydrogenated silicon compounds. II. Role of the hybridization in SiH_n ($n=1, 2$) as compared to CH_n ($n=1, 2$) 174 (1993) 191
Wurfel, B.E., G. Schallmoser, G.M. Lask, J. Agreiter, A. Thoma, R. Schlachta and V.E. Bondybey, Infrared fluorescence and absorption studies of CN: spectra and relaxation in solid rare gases 174 (1993) 255

Yamashita, K., see W. Gabriel 174 (1993) 45
Yoxall, K.R., see P.A. Hatherly 174 (1993) 453

Zakrzewski, V.G., W. von Niessen, A.I. Boldyrev and P. von R. Schleyer, Green function calculation of ionization energies of hypermetallic molecules 174 (1993) 167

Subject Index to Volume 174

Methods

Theoretical

Classical mechanics
Optimal control of classical anharmonic molecules represented with piecewise harmonic potential surfaces: analytic solution and selective dissociation of triatomic systems, M.H. Lissak, J.D. Sensabaugh, C.D. Schwieters, J.G.B. Beumee and H. Rabitz 174 (1993) 1
Nonequilibrium dissociation rates behind strong shock waves: classical model, S.O. Macheret and J.W. Rich 174 (1993) 25
Vibrational chaos: rational tori, separatrices and Lyapunov exponents, M. Joyeux 174 (1993) 157

Quantized field theory
Green function calculation of ionization energies of hypermetallic molecules, V.G. Zakrzewski, W. von Niessen, A.I. Boldyrev and P. von R. Schleyer 174 (1993) 167

Coupling schemes and perturbative treatments
Theoretical study of small hydrogenated silicon compounds. II. Role of the hybridization in SiH_n ($n=1, 2$) as compared to CH_n ($n=1, 2$), C. Winter and P. Millie 174 (1993) 191

Equilibrium statistical mechanics
Reorganization energy of electron transfer in polar liquids. Dependence on reactant size, temperature and pressure, D.V. Matyushov 174 (1993) 199

Non-equilibrium thermodynamic and hydrodynamic theories
Vibrational and electronic excitation of nitric oxide in optical pumping experiments, S. Saupe, I. Adamovich, M.J. Grassi, J.W. Rich and R.C. Bergman 174 (1993) 219

Ab initio schemes for stationary properties
Theoretical rotational–vibrational spectrum of SiH_2 ($X\ ^1A_1$ and $a\ ^3B_1$), W. Gabriel, P. Rosmus, K. Yamashita, K. Morokuma and P. Palmieri 174 (1993) 45
Ab initio CI calculation of K shell absorption spectra in transition metal compounds, G. Fronzoni, P. Decleva and A. Lisini 174 (1993) 57
Theoretical study of a basic process in interstellar nitrogen chemistry: reaction of N with OH, F. Pauzat, Y. Ellinger, G. Berthier, M. Gérin and Y. Viala 174 (1993) 71
Theoretical study of small hydrogenated silicon compounds. I. Theoretical study of the SiH_2 dissociation channels up to 8 eV excitation energy, C. Winter and P. Millie 174 (1993) 177
Theoretical study of small hydrogenated silicon compounds. II. Role of the hybridization in SiH_n ($n=1, 2$) as compared to CH_n ($n=1, 2$), C. Winter and P. Millie 174 (1993) 191

A theoretical study of the $(H_2)_2$ dimer. III. The isotropic potential, P. Wind and I. Røeggen 174 (1993) 345

Computational and simulation methods

Optimal control of classical anharmonic molecules represented with piecewise harmonic potential surfaces: analytic solution and selective dissociation of triatomic systems, M.H. Lissak, J.D. Sensabaugh, C.D. Schwieters, J.G.B. Beumee and H. Rabitz 174 (1993) 1

Scaling analysis of exciton annihilations in highly anisotropic crystals, M. Deal, A. Gharvai, G.L. McPherson, C.E. Martinez and M.F. Herman 174 (1993) 81

Theoretical study of the ground and excited states of ozone in its symmetric nuclear arrangement, A. Banichevich and S.D. Peyerimhoff 174 (1993) 93

On the diffusion mechanism of methane in a cation-free zeolite of type ZK4, S. Fritzsche, R. Haberlandt, J. Kärger, H. Pfeifer and K. Heinzinger 174 (1993) 229

Exponential-α:6 potential parameters from ab initio calculations for atom–molecule interactions, B. Amaee and W. Byers Brown 174 (1993) 351

Influence of external steady source structure on particle distributions and kinetics of diffusion-limited reactions. II. $A+B\rightarrow 0$ simulations, L. Li and R. Kopelman 174 (1993) 367

Quantum-statistical transition probabilities in diabatic 2D-potential surfaces. Influence of coupling in the potential terms, R. Neumann and C. Engler 174 (1993) 377

Molecular dynamics and scattering theory

Optimal control of classical anharmonic molecules represented with piecewise harmonic potential surfaces: analytic solution and selective dissociation of triatomic systems, M.H. Lissak, J.D. Sensabaugh, C.D. Schwieters, J.G.B. Beumee and H. Rabitz 174 (1993) 1

A molecular dynamics investigation of energy transfer efficiency in collisions of diatomic molecules, L.L. Andersson, J. Davidsson and S. Nordholm 174 (1993) 111

The dynamics of some metal–organic and organic molecules in water solution studied by molecular mechanical and molecular dynamical methods, A. Broo 174 (1993) 127

Accurate photoionization cross sections of diatomic molecules by multi-configuration linear response theory, V. Carravetta, Y. Luo and H. Ågren 174 (1993) 141

Calculation of SNP effects in weak magnetic fields, A.M. Osintsev, P.A. Purtov and K.M. Salikhov 174 (1993) 237

The rate of ion-linear dipole capture at extremely low temperatures estimated with the use of the statistical adiabatic channel model, J. Turulski, J. Niedzielski and K. Sakimoto 174 (1993) 387

Chemical reactions in solution: modelling of the delay of solvent synchronism (dielectric friction) along the reaction path of an S_N2 reaction, M. Aguilar, R. Bianco, S. Miertus, M. Persico and J. Tomasi 174 (1993) 397

Experimental

Magnetic resonances

On the diffusion mechanism of methane in a cation-free zeolite of type ZK4, S. Fritzsche, R. Haberlandt, J. Kärger, H. Pfeifer and K. Heinzinger 174 (1993) 229

Microwave spectroscopy

High-resolution laser-induced fluorescence and microwave–ultraviolet double resonance spectroscopy on 1-cyanonaphthalene, G. Berden, W.L. Meerts and W. Kreiner 174 (1993) 247

Infrared spectroscopy

Theoretical rotational–vibrational spectrum of SiH_2 ($X\ ^1A_1$ and $a\ ^3B_1$), W. Gabriel, P. Rosmus, K. Yamashita, K. Morokuma and P. Palmieri 174 (1993) 45

Vibrational and electronic excitation of nitric oxide in optical pumping experiments, S. Saupe, I. Adamovich, M.J. Grassi, J.W. Rich and R.C. Bergman 174 (1993) 219

Infrared fluorescence and absorption studies of CN: spectra and relaxation in solid rare gases, B.E. Wurfel, G. Schallmoser, G.M. Lask, J. Agreiter, A. Thoma, R. Schlachta and V.E. Bondybey 174 (1993) 255

Visible and UV spectroscopy

High-resolution laser-induced fluorescence and microwave–ultraviolet double resonance spectroscopy on 1-cyanonaphthalene, G. Berden, W.L. Meerts and W. Kreiner 174 (1993) 247

High-resolution laser-induced fluorescence study of a cage molecule, 1,4-diazabicyclo[2,2,2]octane, DABCO, D. Consalvo, M. Drabbels, G. Berden, W.L. Meerts, D.H. Parker and J. Reuss 174 (1993) 267

Dissociative excitation of lithium atoms in collisions of electrons with LiCl molecules, Y.M. Smirnov 174 (1993) 277

Radiative and collisional relaxation of a single rovibrational quantum state of I_2: $E(0_g^+)$, $v=8$, $J=56$, W. Ubachs, I. Aben, J.B. Milan, G.J. Somsen, A.G. Stuiver and W. Hogervorst 174 (1993) 285

Fluorine hot atom oxidation of bismuth vapor. A comment on the evaluation of the BiF bond energy, T.C. Devore and J.L. Gole 174 (1993) 409

Two-photon spectroscopy of molecular oxygen, M.P. McCann, C.H. Chen, I. Datskou and S. Evans 174 (1993) 417

Fluorescence spectroscopy

Scaling analysis of exciton annihilations in highly anisotropic crystals, M. Deal, A. Gharvai, G.L. McPherson, C.E. Martinez and M.F. Herman 174 (1993) 81

Infrared fluorescence and absorption studies of CN: spectra and relaxation in solid rare gases, B.E. Wurfel, G. Schallmoser, G.M. Lask, J. Agreiter, A. Thoma, R. Schlachta and V.E. Bondybey 174 (1993) 255

The lowest triplet state of azulene-h_8 and azulene-d_8 in liquid solution. I. Survey, kinetic considerations, experimental technique, and temperature dependence of triplet decay, B. Nickel and D. Klemp 174 (1993) 297

The lowest triplet state of azulene-h_8 and azulene-d_8 in liquid solution. II. Phosphorescence and E-type delayed fluorescence, B. Nickel and D. Klemp 174 (1993) 319

Fluorine hot atom oxidation of bismuth vapor. A comment on the evaluation of the BiF bond energy, T.C. Devore and J.L. Gole 174 (1993) 409

On the source of the anomalous fluorescence of 4-(dialkylamino)benzonitrile in aromatic hydrocarbon solvents: the role of exciplexes, M.C.C. de Lange, D.T. Leeson, K.A.B. van Kuijk, A.H. Huizer and C.A.G.O. Varma 174 (1993) 425

Radiative decay of the $\tilde{C}\ ^2T_2$ state of CF_4^+ measured by threshold photoelectron–fluorescence coincidence spectroscopy, P.A. Hatherly, K. Codling, D.M. Smith, R.P. Tuckett, K.R. Yoxall and J.F.M. Aarts 174 (1993) 453

Photoelectron and Auger spectroscopy

Fragmentation of valence electronic states of CF_4^+ and SF_6^+ studied by threshold photoelectron–photoion coincidence spectroscopy, J.C. Creasey, H.M. Jones, D.M. Smith, R.P. Tuckett, P.A. Hatherly, K. Codling and I. Powis 174 (1993) 441

Laser methods
Vibrational and electronic excitation of nitric oxide in optical pumping experiments, S. Saupe, I. Adamovich, M.J. Grassi, J.W. Rich and R.C. Bergman 174 (1993) 219

Picosecond spectroscopy
On the source of the anomalous fluorescence of 4-(dialkylamino)benzonitrile in aromatic hydrocarbon solvents: the role of exciplexes, M.C.C. de Lange, D.T. Leeson, K.A.B. van Kuijk, A.H. Huizer and C.A.G.O. Varma 174 (1993) 425

Synchrotron spectroscopies
Fragmentation of valence electronic states of CF_4^+ and SF_6^+ studied by threshold photoelectron–photoion coincidence spectroscopy, J.C. Creasey, H.M. Jones, D.M. Smith, R.P. Tuckett, P.A. Hatherly, K. Codling and I. Powis 174 (1993) 441
Radiative decay of the $\tilde{C}\ ^2T_2$ state of CF_4^+ measured by threshold photoelectron–fluorescence coincidence spectroscopy, P.A. Hatherly, K. Codling, D.M. Smith, R.P. Tuckett, K.R. Yoxall and J.F.M. Aarts 174 (1993) 453

Multiple resonance spectroscopy
High-resolution laser-induced fluorescence and microwave–ultraviolet double resonance spectroscopy on 1-cyanonaphthalene, G. Berden, W.L. Meerts and W. Kreiner 174 (1993) 247

Atomic and molecular beam techniques
High-resolution laser-induced fluorescence and microwave–ultraviolet double resonance spectroscopy on 1-cyanonaphthalene, G. Berden, W.L. Meerts and W. Kreiner 174 (1993) 247
High-resolution laser-induced fluorescence study of a cage molecule, 1,4-diazabicyclo[2,2,2]octane, DABCO, D. Consalvo, M. Drabbels, G. Berden, W.L. Meerts, D.H. Parker and J. Reuss 174 (1993) 267
Dissociative excitation of lithium atoms in collisions of electrons with LiCl molecules, Y.M. Smirnov 174 (1993) 277

Time-resolved experiments
Energetic states of positronium in liquids from the study of magnetic field effects and of spin conversion reactions, F. Didierjean, I. Billard, W.F. Magalhaes and G. Duplâtre 174 (1993) 331
Radiative decay of the $\tilde{C}\ ^2T_2$ state of CF_4^+ measured by threshold photoelectron–fluorescence coincidence spectroscopy, P.A. Hatherly, K. Codling, D.M. Smith, R.P. Tuckett, K.R. Yoxall and J.F.M. Aarts 174 (1993) 453

Mass spectrometry
Fragmentation of valence electronic states of CF_4^+ and SF_6^+ studied by threshold photoelectron–photoion coincidence spectroscopy, J.C. Creasey, H.M. Jones, D.M. Smith, R.P. Tuckett, P.A. Hatherly, K. Codling and I. Powis 174 (1993) 441

Objects

Bulk systems

Gases
Nonequilibrium dissociation rates behind strong shock waves: classical model, S.O. Macheret and J.W. Rich 174 (1993) 25

A molecular dynamics investigation of energy transfer efficiency in collisions of diatomic molecules, L.L. Andersson, J. Davidsson and S. Nordholm 174 (1993) 111
Exponential-α:6 potential parameters from ab initio calculations for atom–molecule interactions, B. Amaee and W. Byers Brown 174 (1993) 351
The rate of ion-linear dipole capture at extremely low temperatures estimated with the use of the statistical adiabatic channel model, J. Turulski, J. Niedzielski and K. Sakimoto 174 (1993) 387
Fluorine hot atom oxidation of bismuth vapor. A comment on the evaluation of the BiF bond energy, T.C. Devore and J.L. Gole 174 (1993) 409
Two-photon spectroscopy of molecular oxygen, M.P. McCann, C.H. Chen, I. Datskou and S. Evans 174 (1993) 417

Supersonic beams
Two-photon spectroscopy of molecular oxygen, M.P. McCann, C.H. Chen, I. Datskou and S. Evans 174 (1993) 417

Liquids neat
Energetic states of positronium in liquids from the study of magnetic field effects and of spin conversion reactions, F. Didierjean, I. Billard, W.F. Magalhaes and G. Duplâtre 174 (1993) 331

Liquids mixtures and solutions
The dynamics of some metal–organic and organic molecules in water solution studied by molecular mechanical and molecular dynamical methods, A. Broo 174 (1993) 127
Reorganization energy of electron transfer in polar liquids. Dependence on reactant size, temperature and pressure, D.V. Matyushov 174 (1993) 199
Calculation of SNP effects in weak magnetic fields, A.M. Osintsev, P.A. Purtov and K.M. Salikhov 174 (1993) 237
The lowest triplet state of azulene-h_8 and azulene-d_8 in liquid solution. I. Survey, kinetic considerations, experimental technique, and temperature dependence of triplet decay, B. Nickel and D. Klemp 174 (1993) 297
The lowest triplet state of azulene-h_8 and azulene-d_8 in liquid solution. II. Phosphorescence and E-type delayed fluorescence, B. Nickel and D. Klemp 174 (1993) 319
Energetic states of positronium in liquids from the study of magnetic field effects and of spin conversion reactions, F. Didierjean, I. Billard, W.F. Magalhaes and G. Duplâtre 174 (1993) 331
Chemical reactions in solution: modelling of the delay of solvent synchronism (dielectric friction) along the reaction path of an S_N2 reaction, M. Aguilar, R. Bianco, S. Miertus, M. Persico and J. Tomasi 174 (1993) 397

Crystals
Scaling analysis of exciton annihilations in highly anisotropic crystals, M. Deal, A. Gharvai, G.L. McPherson, C.E. Martinez and M.F. Herman 174 (1993) 81

Surfaces
On the diffusion mechanism of methane in a cation-free zeolite of type ZK4, S. Fritzsche, R. Haberlandt, J. Kärger, H. Pfeifer and K. Heinzinger 174 (1993) 229

Plasmas
Nonequilibrium dissociation rates behind strong shock waves: classical model, S.O. Macheret and J.W. Rich 174 (1993) 25

Microscopic systems

Atoms

Exponential-α: 6 potential parameters from ab initio calculations for atom–molecule interactions, B. Amaee and W. Byers Brown 174 (1993) 351

Molecules (neutral and ionic)

Ab initio CI calculation of K shell absorption spectra in transition metal compounds, G. Fronzoni, P. Decleva and A. Lisini 174 (1993) 57
Theoretical study of a basic process in interstellar nitrogen chemistry: reaction of N with OH, F. Pauzat, Y. Ellinger, G. Berthier, M. Gérin and Y. Viala 174 (1993) 71
The dynamics of some metal–organic and organic molecules in water solution studied by molecular mechanical and molecular dynamical methods, A. Broo 174 (1993) 127
Vibrational chaos: rational tori, separatrices and Lyapunov exponents, M. Joyeux 174 (1993) 157
Theoretical study of small hydrogenated silicon compounds. I. Theoretical study of the SiH_2 dissociation channels up to 8 eV excitation energy, C. Winter and P. Millie 174 (1993) 177
Theoretical study of small hydrogenated silicon compounds. II. Role of the hybridization in SiH_n ($n=1, 2$) as compared to CH_n ($n=1, 2$), C. Winter and P. Millie 174 (1993) 191
High-resolution laser-induced fluorescence study of a cage molecule, 1,4-diazabicyclo[2,2,2]octane, DABCO, D. Consalvo, M. Drabbels, G. Berden, W.L. Meerts, D.H. Parker and J. Reuss 174 (1993) 267
Exponential-α: 6 potential parameters from ab initio calculations for atom–molecule interactions, B. Amaee and W. Byers Brown 174 (1993) 351
Two-photon spectroscopy of molecular oxygen, M.P. McCann, C.H. Chen, I. Datskou and S. Evans 174 (1993) 417

–diatomic

Nonequilibrium dissociation rates behind strong shock waves: classical model, S.O. Macheret and J.W. Rich 174 (1993) 25
A molecular dynamics investigation of energy transfer efficiency in collisions of diatomic molecules, L.L. Andersson, J. Davidsson and S. Nordholm 174 (1993) 111
Accurate photoionization cross sections of diatomic molecules by multi-configuration linear response theory, V. Carravetta, Y. Luo and H. Ågren 174 (1993) 141
Vibrational and electronic excitation of nitric oxide in optical pumping experiments, S. Saupe, I. Adamovich, M.J. Grassi, J.W. Rich and R.C. Bergman 174 (1993) 219
Dissociative excitation of lithium atoms in collisions of electrons with LiCl molecules, Y.M. Smirnov 174 (1993) 277
Radiative and collisional relaxation of a single rovibrational quantum state of I_2: $E(0_g^+)$, $v=8$, $J=56$, W. Ubachs, I. Aben, J.B. Milan, G.J. Somsen, A.G. Stuiver and W. Hogervorst 174 (1993) 285
The rate of ion-linear dipole capture at extremely low temperatures estimated with the use of the statistical adiabatic channel model, J. Turulski, J. Niedzielski and K. Sakimoto 174 (1993) 387
Fluorine hot atom oxidation of bismuth vapor. A comment on the evaluation of the BiF bond energy, T.C. Devore and J.L. Gole 174 (1993) 409

–small polyatomics

Optimal control of classical anharmonic molecules represented with piecewise harmonic potential surfaces: analytic solution and selective dissociation of triatomic systems, M.H. Lissak, J.D. Sensabaugh, C.D. Schwieters, J.G.B. Beumee and H. Rabitz 174 (1993) 1

Theoretical rotational–vibrational spectrum of SiH_2 ($X\ ^1A_1$ and $a\ ^3B_1$), W. Gabriel, P. Rosmus, K. Yamashita, K. Morokuma and P. Palmieri 174 (1993) 45
Theoretical study of the ground and excited states of ozone in its symmetric nuclear arrangement, A. Banichevich and S.D. Peyerimhoff 174 (1993) 93
Green function calculation of ionization energies of hypermetallic molecules, V.G. Zakrzewski, W. von Niessen, A.I. Boldyrev and P. von R. Schleyer 174 (1993) 167
Theoretical study of small hydrogenated silicon compounds. I. Theoretical study of the SiH_2 dissociation channels up to 8 eV excitation energy, C. Winter and P. Millie 174 (1993) 177
Theoretical study of small hydrogenated silicon compounds. II. Role of the hybridization in SiH_n ($n=1, 2$) as compared to CH_n ($n=1, 2$), C. Winter and P. Millie 174 (1993) 191
The rate of ion-linear dipole capture at extremely low temperatures estimated with the use of the statistical adiabatic channel model, J. Turulski, J. Niedzielski and K. Sakimoto 174 (1993) 387
Chemical reactions in solution: modelling of the delay of solvent synchronism (dielectric friction) along the reaction path of an S_N2 reaction, M. Aguilar, R. Bianco, S. Miertus, M. Persico and J. Tomasi 174 (1993) 397
Fragmentation of valence electronic states of CF_4^+ and SF_6^+ studied by threshold photoelectron–photoion coincidence spectroscopy, J.C. Creasey, H.M. Jones, D.M. Smith, R.P. Tuckett, P.A. Hatherly, K. Codling and I. Powis 174 (1993) 441
Radiative decay of the $\tilde{C}\ ^2T_2$ state of CF_4^+ measured by threshold photoelectron–fluorescence coincidence spectroscopy, P.A. Hatherly, K. Codling, D.M. Smith, R.P. Tuckett, K.R. Yoxall and J.F.M. Aarts 174 (1993) 453

–aromatics
High-resolution laser-induced fluorescence and microwave–ultraviolet double resonance spectroscopy on 1-cyanonaphthalene, G. Berden, W.L. Meerts and W. Kreiner 174 (1993) 247
The lowest triplet state of azulene-h_8 and azulene-d_8 in liquid solution. I. Survey, kinetic considerations, experimental technique, and temperature dependence of triplet decay, B. Nickel and D. Klemp 174 (1993) 297
The lowest triplet state of azulene-h_8 and azulene-d_8 in liquid solution. II. Phosphorescence and E-type delayed fluorescence, B. Nickel and D. Klemp 174 (1993) 319
On the source of the anomalous fluorescence of 4-(dialkylamino)benzonitrile in aromatic hydrocarbon solvents: the role of exciplexes, M.C.C. de Lange, D.T. Leeson, K.A.B. van Kuijk, A.H. Huizer and C.A.G.O. Varma 174 (1993) 425

Molecular aggregates

–dimers
A theoretical study of the $(H_2)_2$ dimer. III. The isotropic potential, P. Wind and I. Røeggen 174 (1993) 345

–van der Waals molecules
A theoretical study of the $(H_2)_2$ dimer. III. The isotropic potential, P. Wind and I. Røeggen 174 (1993) 345

–complexes
On the source of the anomalous fluorescence of 4-(dialkylamino)benzonitrile in aromatic hydrocarbon solvents: the role of exciplexes, M.C.C. de Lange, D.T. Leeson, K.A.B. van Kuijk, A.H. Huizer and C.A.G.O. Varma 174 (1993) 425

Free radicals (including hydronium and muonium)
Calculation of SNP effects in weak magnetic fields, A.M. Osintsev, P.A. Purtov and K.M. Salikhov 174 (1993) 237
Infrared fluorescence and absorption studies of CN: spectra and relaxation in solid rare gases, B.E. Wurfel, G. Schallmoser, G.M. Lask, J. Agreiter, A. Thoma, R. Schlachta and V.E. Bondybey 174 (1993) 255
Energetic states of positronium in liquids from the study of magnetic field effects and of spin conversion reactions, F. Didierjean, I. Billard, W.F. Magalhaes and G. Duplâtre 174 (1993) 331

Quasiparticles (including excitions)
Scaling analysis of exciton annihilations in highly anisotropic crystals, M. Deal, A. Gharvai, G.L. McPherson, C.E. Martinez and M.F. Herman 174 (1993) 81

Phenomena

Molecular structure
The dynamics of some metal–organic and organic molecules in water solution studied by molecular mechanical and molecular dynamical methods, A. Broo 174 (1993) 127
Theoretical study of small hydrogenated silicon compounds. I. Theoretical study of the SiH_2 dissociation channels up to 8 eV excitation energy, C. Winter and P. Millie 174 (1993) 177

Vibrations and rotations of molecules
Theoretical rotational–vibrational spectrum of SiH_2 ($X\ ^1A_1$ and $a\ ^3B_1$), W. Gabriel, P. Rosmus, K. Yamashita, K. Morokuma and P. Palmieri 174 (1993) 45
Vibrational chaos: rational tori, separatrices and Lyapunov exponents, M. Joyeux 174 (1993) 157

Electronic structure and states
Theoretical rotational–vibrational spectrum of SiH_2 ($X\ ^1A_1$ and $a\ ^3B_1$), W. Gabriel, P. Rosmus, K. Yamashita, K. Morokuma and P. Palmieri 174 (1993) 45
Ab initio CI calculation of K shell absorption spectra in transition metal compounds, G. Fronzoni, P. Decleva and A. Lisini 174 (1993) 57
Theoretical study of the ground and excited states of ozone in its symmetric nuclear arrangement, A. Banichevich and S.D. Peyerimhoff 174 (1993) 93
Green function calculation of ionization energies of hypermetallic molecules, V.G. Zakrzewski, W. von Niessen, A.I. Boldyrev and P. von R. Schleyer 174 (1993) 167
Theoretical study of small hydrogenated silicon compounds. I. Theoretical study of the SiH_2 dissociation channels up to 8 eV excitation energy, C. Winter and P. Millie 174 (1993) 177
Theoretical study of small hydrogenated silicon compounds. II. Role of the hybridization in SiH_n ($n=1, 2$) as compared to CH_n ($n=1, 2$), C. Winter and P. Millie 174 (1993) 191
Fragmentation of valence electronic states of CF_4^+ and SF_6^+ studied by threshold photoelectron–photoion coincidence spectroscopy, J.C. Creasey, H.M. Jones, D.M. Smith, R.P. Tuckett, P.A. Hatherly, K. Codling and I. Powis 174 (1993) 441
Radiative decay of the $\tilde{C}\ ^2T_2$ state of CF_4^+ measured by threshold photoelectron–fluorescence coincidence spectroscopy, P.A. Hatherly, K. Codling, D.M. Smith, R.P. Tuckett, K.R. Yoxall and J.F.M. Aarts 174 (1993) 453

Molecular interactions
A theoretical study of the $(H_2)_2$ dimer. III. The isotropic potential, P. Wind and I. Røeggen 174 (1993) 345
Exponential-α:6 potential parameters from ab initio calculations for atom–molecule interactions, B. Amaee and W. Byers Brown 174 (1993) 351

Energy transfer processes
A molecular dynamics investigation of energy transfer efficiency in collisions of diatomic molecules, L.L. Andersson, J. Davidsson and S. Nordholm 174 (1993) 111
Vibrational and electronic excitation of nitric oxide in optical pumping experiments, S. Saupe, I. Adamovich, M.J. Grassi, J.W. Rich and R.C. Bergman 174 (1993) 219
Radiative and collisional relaxation of a single rovibrational quantum state of I_2: $E(0_g^+)$, $v=8$, $J=56$, W. Ubachs, I. Aben, J.B. Milan, G.J. Somsen, A.G. Stuiver and W. Hogervorst 174 (1993) 285

Molecular photophysical processes
Theoretical study of the ground and excited states of ozone in its symmetric nuclear arrangement, A. Banichevich and S.D. Peyerimhoff 174 (1993) 93
The lowest triplet state of azulene-h_8 and azulene-d_8 in liquid solution. I. Survey, kinetic considerations, experimental technique, and temperature dependence of triplet decay, B. Nickel and D. Klemp 174 (1993) 297
The lowest triplet state of azulene-h_8 and azulene-d_8 in liquid solution. II. Phosphorescence and E-type delayed fluorescence, B. Nickel and D. Klemp 174 (1993) 319
On the source of the anomalous fluorescence of 4-(dialkylamino)benzonitrile in aromatic hydrocarbon solvents: the role of exciplexes, M.C.C. de Lange, D.T. Leeson, K.A.B. van Kuijk, A.H. Huizer and C.A.G.O. Varma 174 (1993) 425

Intramolecular dynamics
The dynamics of some metal–organic and organic molecules in water solution studied by molecular mechanical and molecular dynamical methods, A. Broo 174 (1993) 127
Vibrational chaos: rational tori, separatrices and Lyapunov exponents, M. Joyeux 174 (1993) 157

–vibrational energy redistribution (including vibrational dissociation)
Infrared fluorescence and absorption studies of CN: spectra and relaxation in solid rare gases, B.E. Wurfel, G. Schallmoser, G.M. Lask, J. Agreiter, A. Thoma, R. Schlachta and V.E. Bondybey 174 (1993) 255

Luminescence spectra, yields and lifetimes
The lowest triplet state of azulene-h_8 and azulene-d_8 in liquid solution. I. Survey, kinetic considerations, experimental technique, and temperature dependence of triplet decay, B. Nickel and D. Klemp 174 (1993) 297
The lowest triplet state of azulene-h_8 and azulene-d_8 in liquid solution. II. Phosphorescence and E-type delayed fluorescence, B. Nickel and D. Klemp 174 (1993) 319

Multiphoton phenomena
Two-photon spectroscopy of molecular oxygen, M.P. McCann, C.H. Chen, I. Datskou and S. Evans 174 (1993) 417

Reactions (including dissociation)
Theoretical study of a basic process in interstellar nitrogen chemistry: reaction of N with OH, F. Pauzat, Y. Ellinger, G. Berthier, M. Gérin and Y. Viala 174 (1993) 71
Influence of external steady source structure on particle distributions and kinetics of diffusion-limited reactions. II. A+B→0 simulations, L. Li and R. Kopelman 174 (1993) 367
Quantum-statistical transition probabilities in diabatic 2D-potential surfaces. Influence of coupling in the potential terms, R. Neumann and C. Engler 174 (1993) 377
Fluorine hot atom oxidation of bismuth vapor. A comment on the evaluation of the BiF bond energy, T.C. Devore and J.L. Gole 174 (1993) 409

–gas phase
Nonequilibrium dissociation rates behind strong shock waves: classical model, S.O. Macheret and J.W. Rich 174 (1993) 25
Theoretical study of a basic process in interstellar nitrogen chemistry: reaction of N with OH, F. Pauzat, Y. Ellinger, G. Berthier, M. Gérin and Y. Viala 174 (1993) 71
Dissociative excitation of lithium atoms in collisions of electrons with LiCl molecules, Y.M. Smirnov 174 (1993) 277
The rate of ion-linear dipole capture at extremely low temperatures estimated with the use of the statistical adiabatic channel model, J. Turulski, J. Niedzielski and K. Sakimoto 174 (1993) 387

–condensed phase
Calculation of SNP effects in weak magnetic fields, A.M. Osintsev, P.A. Purtov and K.M. Salikhov 174 (1993) 237
Quantum-statistical transition probabilities in diabatic 2D-potential surfaces. Influence of coupling in the potential terms, R. Neumann and C. Engler 174 (1993) 377
Chemical reactions in solution: modelling of the delay of solvent synchronism (dielectric friction) along the reaction path of an S_N2 reaction, M. Aguilar, R. Bianco, S. Miertus, M. Persico and J. Tomasi 174 (1993) 397

–photochemical
Theoretical study of the ground and excited states of ozone in its symmetric nuclear arrangement, A. Banichevich and S.D. Peyerimhoff 174 (1993) 93

Tunneling
Quantum-statistical transition probabilities in diabatic 2D-potential surfaces. Influence of coupling in the potential terms, R. Neumann and C. Engler 174 (1993) 377

Electron transfer
Reorganization energy of electron transfer in polar liquids. Dependence on reactant size, temperature and pressure, D.V. Matyushov 174 (1993) 199
Quantum-statistical transition probabilities in diabatic 2D-potential surfaces. Influence of coupling in the potential terms, R. Neumann and C. Engler 174 (1993) 377

Positron annihilation
Energetic states of positronium in liquids from the study of magnetic field effects and of spin conversion reactions, F. Didierjean, I. Billard, W.F. Magalhaes and G. Duplâtre 174 (1993) 331

Ionization (including Rydberg states)
Accurate photoionization cross sections of diatomic molecules by multi-configuration linear response theory, V. Carravetta, Y. Luo and H. Ågren 174 (1993) 141
Green function calculation of ionization energies of hypermetallic molecules, V.G. Zakrzewski, W. von Niessen, A.I. Boldyrev and P. von R. Schleyer 174 (1993) 167

Molecular motion (including diffusive)
On the diffusion mechanism of methane in a cation-free zeolite of type ZK4, S. Fritzsche, R. Haberlandt, J. Kärger, H. Pfeifer and K. Heinzinger 174 (1993) 229

Isotopic effects
Infrared fluorescence and absorption studies of CN: spectra and relaxation in solid rare gases, B.E. Wurfel, G. Schallmoser, G.M. Lask, J. Agreiter, A. Thoma, R. Schlachta and V.E. Bondybey 174 (1993) 255

Fluctuations and noise
Reorganization energy of electron transfer in polar liquids. Dependence on reactant size, temperature and pressure, D.V. Matyushov 174 (1993) 199

Thermodynamic and transport properties
On the diffusion mechanism of methane in a cation-free zeolite of type ZK4, S. Fritzsche, R. Haberlandt, J. Kärger, H. Pfeifer and K. Heinzinger 174 (1993) 229

Structure of solids and liquids
Reorganization energy of electron transfer in polar liquids. Dependence on reactant size, temperature and pressure, D.V. Matyushov 174 (1993) 199